

Not official

Claim submitted for discussion purposes only.

A computer implemented method for configuring [the] molecular structures derived from reactant molecules into a [standardized] representative conformation enabling comparison between the structures of shape related properties, comprising the following steps:

- a) defining topomeric alignment rules;
- b) obtaining, or generating from two dimensional (2D) structural information, the three dimensional (3D) configuration of the molecular structures [represented by the three dimensional coordinates of the atoms] - *concord* comprising the structures] and
- c) repositioning the relative positions of atoms in the structures by adjusting torsions according to the topomeric alignment rules

wherein a single, consistent, and unambiguous aligned topomeric conformation is produced for each structure.

for record only as discussion